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13. ABSTRACT (Maximum 200 Words)

The research activities are focused on modeling of polymeric liquid crystal (LCP) flows. We first summarizes our comprehensive studies on the shear and elongational flow with an imposed velocity field. This includes a complete characterization of the orientational equilibria and their bifurcation behavior as well as the detailed study on the orientation dynamics with respect to both types of flows. In particular, biaxial patterns and their dynamics are treated carefully. We then report on the work on the modeling of fiber spinning processes of thermotropic liquid crystal polymers, where new models along with an extensive study for fiber flows of thermotropic liquid crystals are presented. The study on the influence of microstructure on the capillary instability of liquid crystal jets follows. Finally, we report on some long wave stability analysis for ideal liquid jets of LCPs and the progress on some ongoing projects.

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Final Technical Report

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Principal Investigator: Qi Wang

This is the final technical report to AFOSR summarizing the research activities of mine during the period from April 1, 1996 to December 31, 1998 while partially supported by the AFOSR under the grant F49620-96-0131. In this period, my research activities are mainly focused on modeling of polymeric liquid crystal flows. The research efforts are primarily directed to the understanding of the flow-orientation coupling in the liquid with microstructures using orientation (conformation) tensor based models. In the following, I tersely describe the work done in this direction and pertinent directions.

A. Orientational patterns in steady shear flows and their orientational stability

It has been a tradition in the rheological research that rheological properties of the liquid in question are studied first under imposed shear flow field. This approach is simplified though. But, it indeed gives rise to the exact steady state solution to the governing equation system of the flow in steady states. Using an approximate Doi type theory, we studied the orientational dynamics with respect to an imposed velocity field consistent with the shear flow. We were able to calculate all the steady states of the orientation tensor equation which governs the evolution of the second order orientation tensor. For the first time, we clearly identified the orientation patterns given by the Doi type theory as biaxial. The variation of the orientation patterns with respect to the shear rate is studied in great detail. The bifurcation behavior of the steady states with respect to both a dimensionless concentration parameter as well as the shear rate is presented. Furthermore, we give a precise description on the stability of the steady states residing in a 3-dimensional invariant space in the context of the 5-D orientation tensor space, which clarifies some mischaracterizations published in the previous literatures.

B. Comparative studies on approximate Doi type theories using closure approximations

The Doi type theory is a kinetic theory. At every space and time location, a probability density function on a sphere must be solved in order to characterize the average molecular

orientation. An analytical study for flows of liquid crystal polymers proves to be extremely tedious and often intractable with this type of theory. Consequently, several attempts have been made to derive approximate liquid crystal theories in which the probability density function is not explicitly involved. There are three approximate schemes that have been applied to obtain approximate theories. They are the Doi, Hinch-Leal 1 and 2 closure approximations. In this study, we exhaustively compare the approximate theories obtained by applying all the three closures on a Doi type theory developed by Bhave et al. in elongational and slender fiber flows. We found that so long as the flow-interaction term is approximated by the Doi closure, the prolate solutions are in good agreement with the corresponding exact solutions. If, in addition, we restrict to the Doi and Hinch-Leal 2 approximation to the molecular-molecular interaction terms in the kinetic theory, the results are in very good agreement with the exact theory. The best overall approximate theory is found to be obtained by using Doi on flow-interaction and Hinch-Leal 2 on the molecular-molecular interaction term. This study assures the usefulness, especially, the legitimacy of using the approximate theory in fiber flows.

C. 1-D fiber flows of liquid crystal polymers

This is a joint work with Prof. M. Greg Forest and Dr. Hong Zhou of the University of North Carolina at Chapel Hill and Prof. S. E. Bechtel of the Ohio State University. As a continuing effort to study fiber spinning of liquid crystalline polymers, we derived 1-D asymptotic model equations from the 3-D approximate BMAB theory. Using the 1-D theory, we effectively explored the effect of orientation coupling to the flow in steady states of fiber spinning processes and their stability with respect to ambient disturbances. We reassured the fiber flow is nearly uniaxial and exhibiting converging director distribution along the spinning line and discovered that the more stable steady state favors less ordered upstream orientations. In a most recent paper, we extended the study to thermotropic liquid crystals, where phase transition may take place as temperature varies. One of the upshot of the study is that the average internal orientation is less sensitive to the detailed form of the intermolecular potential (bulk free energy) in this flow. Further studies in this direction such as the measurement of certain physical parameters in the theory needs to be carried out in the near future.

D. Couette flows of liquid crystal polymers

This is a fundamental study on the orientational dynamics of liquid crystal polymers in a simple nonlinear flow field. We looked into the flow-orientation interaction in a flow field between two rotating concentric cylinders. By using the BMAB approximate theory obtained from Doi closure approximation, we mainly examined the orientational patterns in the flow-aligning regime of liquid crystal polymers. We found that the steady states may be flow-aligning, where the major director tends to align in the direction of the flow, log-rolling, the major director is fixed in the direction of the angular velocity, and a mixed regime, where the flow aligning behavior dominates near the wall of the inner cylinder while log-rolling phenomena prevails near the outer cylinder. This mixed behavior has been wrongly interpreted as formation of defects. Due to our biaxial representation of the orientation tensor, this de-

ceptive phenomenon is found merely a change of orientation pattern rather than formation of defects.

E. Orientation-induced growthrate reduction in jet flows of liquid crystal polymers

We generalized the classical Rayleigh stability analysis to free surface jet flows of liquid crystal polymers. The model we used is a generalized Doi model along with a modified free surface kinetic boundary condition, in which microstructure dependent surface tension is implemented through a novel surface energy term. We discovered analytically that the unstable band of wave numbers for the prolate steady states may be narrowed due to the microstructure-dependent surface tension, in the meantime, the growthrate curves is lowered as well. The growthrate curve lowers to zero as the anisotropic drag coefficient decreases toward zero if the orientation energy dominates the surface tension energy. The zero anisotropic limit corresponds to a hyper-anisotropic liquid crystal. If the surface energy dominates the orientation energy, the growthrate curve is bounded below by a positive curve, which is given by the hyper-anisotropic limit. The cutoff wave number is explicitly given by $k_{cutoff} = \sqrt{\frac{1}{1+2\xi s^2}\frac{1}{R_0}}$, where ξ measures the anisotropic contribution to the surface energy, s measures the degree of orientation in the jet equilibrium and R_0 is the radius of the equilibrium jet. All oblate steady states and isotropic states in the range of large polymer concentration are unstable to all wave numbers.

F. Thermal-mechanically consistent theory

In order to model the expansion cooling phenomenon in pressure driven polymer flows, Cao et al. developed a thermal-mechanically consistent theory by postulating density a function of the temperature. However, I found this theory is illposed near the constant equilibrium, where the Hadamard instability prevails. In collaboration with F. Ronney of University of California, S. Bechtel of OSU, we analyzed the pathological behavior of this theory rigorously and gave a partial fix to the theory. We found when the density is postulated as a function of entropy instead of temperature, the theory becomes well-posed. We also illustrated the source for the illposedness in the neighborhood of the constant equilibrium by examining the the free energy and internal energy there.

G. Study of universal solutions of axisymmetric cylindrical liquid jets

Motivated by the work of Segur on inviscid and viscous liquid jets and early work of Helfrich on membranes, the PI has found two universal solution families for any jet flow of simple fluids, including many viscoelastic fluids and liquid crystal polymers. The linearized stability for slender jets has been carried out using 1-D models for several well know materials such as isotropic viscoelastic fluids and liquid crystal polymers. For the LCP materials, flow-orientation interaction is accounted for in the bulk as well as free surface. The stability of the jet of a varying radius as well as the jet of a constant radius under the influence of gravity is established provided the axial force is negative. This may be entirely due to the

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microstructure for the liquid crystal polymer.

H. Construction of the steady states and their stability in imposed elongational flow field

Parallel to the study of steady states in shear flows of LCPs, the PI, M. G. Forest and H. Zhou of Univ. of North Carolina Chapel Hill studied the formation of steady states in an imposed elongational flow field. We showed and classified all steady states and their stability properties in the 5-D orientation tensor space. We even proved that the only equilibrium, at the absence of a flow field, is uniaxial as far as the Doi type theory is concerned. A comprehensive bifurcation analysis with respect to the elongational rate as well as the dimensionless concentration was conducted. Some stable biaxial orientation patterns are characterized explicitly. Hopefully, further experimental work will be able to confirm their existence.

I. Other pertinent works

In addition to the above mentioned works, I also looked into the well-posedness of the Doi type theory near flow equilibrium together with M. G. Forest. We characterized the distinctive directional instability in the flow equilibrium with the so called oblate uniaxial equilibrium. We also investigated the regularizing effect of viscosity, spatial diffusion and long-range intermolecular interaction. While the long range intermolecular interaction is included in the model, we then examined the formation of periodic solutions. The existence of the periodic patterns and their stability in shear as well as Poiseuille flows is currently under investigation.

J. Ongoing projects

(1). In collaboration with Prof. M. Carme Calderer and Chun Liu of Penn State University, we are developing a general biaxial theory for liquid crystal polymers that may exhibit smectic structures. We combine the continuum mechanics approach with that of the Landau-deGennes. We have already established the framework for the theory. Detailed analyses for liquid crystal polymers of this kind in shear flows are currently underway.
(2). I am studying the formation of texture in steady state Poiseuille flows using the Doi type biaxial theory for spatially nonhomogeneous liquid crystals. This basic study will lay the foundation for more daring study on the variation of the defects under nonlinear flow fields.

Finally, I tabulate the papers published, accepted and in review during the reported period in the following.

K. Papers published

1. Q. Wang, "Biaxial Steady States and Their Stability in Shear Flows of Liquid Crystal Polymers", *Journal of Rheology* 41, 1997, pp. 943–970

2. Q. Wang, "Comparative Studies on Closure Approximations in Flows of Liquid Crystal

Polymers. I. Elongational Flows", *Journal of Non-Newtonian Fluid Mechanics* 72, 141-162, 1997.

3. Q. Wang, "Comparative Studies on Closure Approximations in Flows of Liquid Crystal Polymers. II. Fiber Flows", *Journal of Non-Newtonian Fluid Mechanics* 72, 163-185, 1997.

4. M. G. Forest, Q. Wang, and S. E. Bechtel, "1 Dimensional Isothermal Spinning Models for Liquid Crystalline Polymer Fibers", *Journal of Rheology* 41, 1997, pp. 821-850.

5. M. G. Forest and Q. Wang, "Anisotropic microstructure-induced reduction of the Rayleigh instability for liquid crystalline polymers", *Physical Letters A* 245 (1998), pp. 518-526.

6. Q. Wang, "Couette Flows of Liquid Crystal Polymers", *Rheology and Fluid Mechanics of Nonlinear Materials*, edited by D. A. Siginer and S. G. Advani, AMD-Vol. 217, ASME, 1996, pp. 109-122.

7. Q. Wang, M. G. Forest and H. Zhou, "Dynamics of free surface and pure elongational flows of liquid crystalline polymers", *Rheology and Fluid Mechanics of Nonlinear Materials*, edited by D. A. Siginer and D. DeKee, FED-Vol 246, MD-Vol 81, ASME, New York, 1998, pp. 101-114.

L. **Papers accepted**

1. S. E. Bechtel, M. G. Forest, Q. Wang and Hong Zhou, "Free Surface Viscoelastic Fibers and Jets", *Advances in the Flow and Rheology of Non-Newtonian Fluids*, Elsevier Science, to appear 1998.

2. M. G. Forest and Q. Wang, "The Role of Microstructure in Taming the Rayleigh Instability of Cylindrical Jets", to appear *Physica D*, 1998.

3, Q. Wang and M. G. Forest, "Near-equilibrium dynamics of Doi models for liquid crystal polymer flows: catastrophic and regularized behavior", to appear *Journal of Non-Newtonian Fluid Mechanics*, 1998.

M. **Papers submitted**

1. M. G. Forest, H. Zhou and Q. Wang, "1-D nonisothermal fiber spinning models for thermotropic liquid crystals", submitted to *Siam Journal on Applied Math*, 1997.

2. M. G. Forest, H. Zhou and Q. Wang, "Fiber Spinning of thermotropic liquid crystal polymers: steady states and stability", submitted to *Journal of Rheology*, 1998.

3. Q. Wang, "Illposedness in Thermomechanically consistent constrained theory for materials with prescribed temperature-dependent density", submitted to *Journal of Applied Mechanics*, 1998.

4. Q. Wang, "Special cylindrical free surface jets of liquid crystalline polymers and their stability", submitted to *Journal of Non-Newtonian Fluid Mechanics*, 1998.

5. Q. Wang, "Influence of Surface Elasticity on Capillary Instability of Cylindrical Jets of Liquid Crystalline Polymers", submitted to Physics of Fluids, 1998.

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